Author Index to Volume 1

Allinger, N. L.: Graphite: A Molecular Mechanics Treatment, with Sprague, J. T., 257
—, and Profeta, S., Jr.: The Torsional Potential Function for *n*-Butane, 181
—, Burkert, V., and Profeta, S., Jr.: *Ab Initio* Calculations of the Rotational Potential Functions for Propylamine and Ethylmethylamine, 281
—, Yuh, Y., and Sprague, J. T.: The Structures and Energies of Some Unsaturated Four-Membered Ring Carbocycles, 30

Balaban, A. T.: Graph Theoretical Characterization and Computer Generation of Certain Carcinogenic Benzenoid Hydrocarbons and Identification of Bay Regions, with Balasubramanian, K., Kaufman, J. J., and Koski, W. S., 149
Balasubramanian, K., Kaufman, J. J., Koski, W. S., and Balaban, A. T.: Graph Theoretical Characterization and Computer Generation of Certain Carcinogenic Benzenoid Hydrocarbons and Identification of Bay Regions, 149
Ball, J. R., and Thomson, C.: Quantum Chemical Investigations of Charge Transfer Interactions in Relation to the Electronic Theory of Cancer. II, 275
—, and —: Quantum Chemical Investigations of Charge Transfer Interactions in Relation to the Electronic Theory of Cancer. IV. The Interaction of Formamide and the Enol Tautomers of Several Glyoxals, 400
Bartell, L. S.: A Pseudopotential SCF-MO Study of Te_4^{2-}, with Rothman, M. J., Ewig, C. S., and Van Wazer, J. R., 64
Bauld, N. L.: A Theoretical Comparison of Cationic and Anionic Homoaromaticity: Reinforcement of Cationic Homoaromaticity by σ-Nonclassical Effects, with Wirth, D., 189
Bock, C. W.: An *Ab initio* Study of the Geometry and Energy of Six Planar Conformers of β-Hydroxyacrolein, with George, P., and Trachtman, M., 373
—, Trachtman, M., and George, P.: An *Ab Initio* Study of the Geometry, Harmonic and Anharmonic Force Fields, and Fundamental Vibrational Frequencies of *Cis*- and *Trans*-Thiolformic Acid, 167
Böhm, M. C., and Gleiter, R.: INDO-Type Calculations on the Ground State and Various Ionic States of Transition Metal Tricarbonyls, 407
Borden, W. T.: A Theoretical Study of Paths for Decomposition and Rearrangement of Dihydroxycarbene, with Feller, D., and Davidson, E. R., 158
Braun-Keller, E.: Systemic Synthesis Design. 8. Generation of Reaction Sequences, with Hendrickson, J. B., 323
Buemi, G.: Spectroscopic CNDO/CI Study of Some Cyclic Polyenes, with Zuccarello, F., and Raudino, A., 341
Burkert, U.: Applications of Molecular Mechanics Calculations in Carbohydrate Chemistry. I. Conformational and Constitutional Equilibria of Tetraoxabicyclo[4.4.0]- and -[5.3.0]decanes, Bicyclic Diacetals of Alditols, 192
—: *Ab Initio* Calculations of the Rotational Potential Functions for Propylamine and Ethylmethylamine, with Allinger, N. L., and Profeta, S., Jr., 281
—: *Ab Initio* Calculations of the Rotational Potential Functions for Propylamine and Ethyl Methyl Ether, 285

Chesnut, D. B., and Whitehurst, F. W.: A Simplex Optimized INDO Calculation of ^{13}C Chemical Shifts in Hydrocarbons, 36
Collins, J. B., and Streitwieser, A., Jr.: Integrated Spatial Electron Populations in Molecules: Application to Simple Molecules, 81
Cooper, I. L., and Pounder, C. N. M.: A Systematic CI Procedure with Modified Virtual Orbitals, 69
Csizmadia, I. G.: Conformational Energy Surfaces of Triplet-State Isomeric Methyloxiranes, with DeMaré, G. R., Peterson, M. R., and Strausz, O. P., 141

Davidson, E. R.: A Theoretical Study of Paths for Decomposition and Rearrangement of Dihydroxycarbene, with Feller, D., and Borden, W. T., 158
De, B. R., and Sannigrahi, A. B.: A Comparative Study of the Structure and Bonding of HOO, HOS, HSO, and HSS Radicals by CNDO/2 and INDO Methods, 334
DeMaré, G. R., Peterson, M. R., Csizmadia, I. G., and Strausz, O. P.: Conformational Energy Surfaces of Triplet-State Isomeric Methyloxiranes, 141
de Oliveira, M.: The Electrostatic Potential of Yeast $tRNA^{Phe}$. II. The Potentials of the Phosphate Groups in Their Various Conformational States, with Lavery, R., and Pullman, B., 301

Ewig, C. S.: A Pseudopotential SCF-MO Study of Te_4^{2-}, with Rothman, M. J., and Bartell, L. S., and Van Wazer, J. R., 64

Feller, D., Borden, W. T., and Davidson, E. R.: A Theoretical Study of Paths for Decomposition and Rearrangement of Dihydroxycarbene, 158

George, P.: An *Ab Initio* Study of the Geometry, Harmonic and Anharmonic Force Fields, and Fundamental Vibrational Frequencies of *Cis*- and *Trans*-Thiolformic Acid, with Bock, C. W., and Trachtman, M., 167
—, Bock, C. W., and Trachtman, M.: An *Ab Initio* Study of the Geometry and Energy of Six Planar Conformers of β-Hydroxyacrolein, 373
Gleiter, R.: INDO-Type Calculations on the Ground State and Various Ionic States of Transition Metal Tricarbonyls, with Böhm, M. C., 407
Gosavi, R. K.: A Note on Density Matrix Extrapolation and Multiple Solutions of the Unrestricted Hartree–Fock Equations, with Mezey, P. G., and Strausz, O. P., 178

Hall, D., and Headford, C. E. L.: An Analysis of the Molecular Packing of Maleic Hydrazide, 261
—, and Wood, M. K.: Prediction of the Crystal

Structure of a Cyclic Tetrapeptide, 368
Headford, C. E. L.: An Analysis of the Molecular Packing of Maleic Hydrazide, with Hall, D., 261
Hendrickson, J. B., and Braun-Keller, E.: Systematic Synthesis Design. 8. Generation of Reaction Sequences, 323
Hilal, R.: Molecular Charge Distribution and Chemical Binding in Five-Membered Heterocycles. I, 348
—: Localized Molecular Orbitals and Chemical Binding in Five-Membered Heterocycles. II, 358
Hinchliffe, A.: The Barrier to Internal Rotation in Ge_2H_6, 185
Hinde, A. L., Pross, A., and Radom, L.: A Theoretical Approach to Substituent Effects. Interactions between Directly Bonded Groups in the Neutrals X—NH_2, X—OH, and X—F and the Anions X—NH^- and X—O^-, 118
Hong, S. H.: Atomic X_α Calculations Based on $E^{HFS}(\alpha) = E^{exp}$, with Tseng, T. J., and Whitehead, M. A., 88
Huzinaga, S.: A Systematic Preparation of New Contracted Gaussian-Type Orbital Sets. III. Second-Row Atoms from Li through Ne, with Tatewaki, H., 205

Iroff, L. D.: On the Gearing of Methyl Groups in Hexamethylbenzene, 76

Jeffrey, G. A., and Taylor, R.: The Application of Molecular Mechanics to the Structures of Carbohydrates, 99

Karplus, M.: A Method for Constrained Energy Minimization of Macromolecules, with van Gunsteren, W. F., 266
Kaufman, J. J.: Graph Theoretical Characterization and Computer Generation of Certain Carcinogenic Benzenoid Hydrocarbons and Identification of Bay Regions, with Balasubramanian, K., Koski, W. S., and Balaban, A. T., 149
Kausch, M., and von Ragué Schleyer, P.: Isomeric Structures of Protonated Ozone: A Theoretical Study, 94
Kelsey, D. R.: Orbital Topology. I. A Basic Topological Model for Chemical Systems, an Orbital Mapping Technique, and Analyses of Model, Thermal Electrocyclic Reactions, 3
—: Orbital Topology. II. Orbital Mapping of Unsymmetrical Molecules. A Survey of the Thermal Isomerizations of Dewar Isomers of Isoelectronically Substituted Benzenes, Cyclopentadienes, and Cyclopentadienyl Ions, 21
Kinch, R. J.: Conformational Analysis of Proteins: Algorithms and Data Structures for Array Processing, with Pottle, C., Pottle, M. S., Tuttle, R. W., and Scheraga, H. A., 46
Koski, W. S.: Graph Theoretical Characterization and Computer Generation of Certain Carcinogenic Benzenoid Hydrocarbons and Identification of Bay Regions, with Balasubramanian, K., Kaufman, J. J., and Balaban, A. T., 149
Krishnan, R.: Small Elemental Clusters. I. The Structures of Be_2, Be_3, Be_4, and Be_5, with Whiteside, R. A., Pople, J. A., Krogh-Jespersen, M.-B., von Ragué Schleyer, P., and Wenke, G., 307
Krogh-Jespersen, M.-B.: Small Elemental Clusters. I. The Structures of Be_2, Be_3, Be_4, and Be_5, with Whiteside, R. A., Krishnan, R., Pople, J. A., von Ragué Schleyer, P., and Wenke, G., 307

Latajka, A., Szezesniak, M. M., Ratajczak, H., and Orville-Thomas, W. J.: Properties of Strong Hydrogen-Bonded Systems. II. *Ab initio* SCF-MO Study of the Hydrogen Bond between Nitric Acid and Ammonia, 417
Lavery, R., de Oliveira, M., and Pullman, B.: The Electrostatic Potential of Yeast $tRNA^{Phe}$. II. The Potentials of the Phosphate Groups in Their Various Conformational States, 301

McManus, S. P., Smith, M. R., Smith, M. B., and Shafer, S. G.: Evaluation of MINDO/3 Calculated Structures. II. Branching Errors in Alkanes and Cycloalkanes, 233
Meyer, A. Y.: Molecular Mechanics of Organic Halides. III. Flourinated Olefins, 111
Meyer, E. F., Jr.: The Computational Application of the Cahn–Ingold–Prelog Rules 1 and 2, 229
Mezey, P. G., and Rao, Ch. V. S. R.: On the Relative Importance of Core and Valence Shell Representation in the Calculation of Conformational Energies Using Small Gaussian Basis Sets, 134
—, Strausz, O. P., and Gosavi, R. K.: A Note on Density Matrix Extrapolation and Multiple Solutions of the Unrestricted Hartree–Fock Equations, 178
Mishra, P. C.: Electronic Structure of Benzaldehyde: A Comparative Study of the Lowest Excited Singlet $\pi^* \leftarrow \pi$ and $\pi^* \leftarrow n$ States, with Srivastava, S. K., 288

Norman, J. G., Jr., and Ryan, P. B.: Metal–Metal Bond Energies in Mo_2, $Mo_2Cl_8^{4-}$, and $Mo_2(O_2CH)_4$, 59

Orville-Thomas, W. J.: Properties of Strong Hydrogen-Bonded Systems. II. *Ab initio* SCF-MO Study of the Hydrogen Bond between Nitric Acid and Ammonia, with Latajka, A., Szezsniak, M. M., and Ratajczak, H., 417

Peoples, H. A.: The Electronic Structure and Optical Activity of Conjugated Dienes: 1,3-Butadiene and α- and β-Phellandrene, with Rauk, A., 240
Peterson, M. R.: Conformational Energy Surfaces of Triplet-State Isomeric Methyloxiranes, with DeMaré, G. R., Csizmadia, I. G., and Strausz, O. P., 141
Pople, J. A.: Small Elemental Clusters. I. The Structures of Be_2, Be_3, Be_4, and Be_5, with Whiteside, R. A., Krishnan, R., Krogh-Jespersen, M.-B., von Ragué Schleyer, P., and Wenke, G., 307
—, Seeger, U., Seeger, R., and von Ragué Schleyer, P.: The Structure of Carbon Trioxide, 199
Pottle, C., Pottle, M. S., Tuttle, R. W., Kinch, R. J., and Scheraga, H. A.: Conformational Analysis of

Proteins: Algorithms and Data Structures for Array Processing, 46

Pottle, M. S.: Conformational Analysis of Proteins: Algorithms and Data Structures for Array Processing, with Pottle, C., Tuttle, R. W., Kinch, R. J., and Scheraga, H. A., 46

Pounder, C. N. M.: A Systematic CI Procedure with Modified Virtual Orbitals, with Cooper, I. L., 69

Profeta, S., Jr.: The Torsional Potential Function for *n*-Butane, with Allinger, N. L., 181

—: *Ab Initio* Calculations of the Rotational Potential Functions for Propylamine and Ethylmethylamine, with Allinger, N. L., and Burkert, U., 281

Pross, A.: A Theoretical Approach to Substituent Effects. Interactions between Directly Bonded Groups in the Neutrals X—NH_2, X—OH, and X—F and the Anions X—NH^- and X—O^-, with Hinde, A. L., and Radom, L., 118

—, and Radom, L.: A Theoretical Approach to Substituent Effects. Structural Consequences of Electrostatic and Orbital Interactions in Model Mono- and Disubstituted Methanes, 295

Pullman, B.: The Electrostatic Potential of Yeast $t\mathrm{RNA}^{\mathrm{Phe}}$. II. The Potentials of the Phosphate Groups in Their Various Conformational States, with Lavery, R., and de Oliveira, M., 301

Radom, L.: A Theoretical Approach to Substituent Effects. Interactions between Directly Bonded Groups in the Neutrals X—NH_2, X—OH, and X—F and the Anions X—NH^- and X—O^-, with Hinde, A. L., and Pross, A., 118

—: A Theoretical Approach to Substituent Effects. Structural Consequences of Electrostatic and Orbital Interactions in Model Mono- and Disubstituted Methanes, with Pross, A., 295

Randić, M.: Random Walks and Their Diagnostic Value for Characterization of Atomic Environment, 386

Rao, Ch. V. S. R.: On the Relative Importance of Core and Valence Shell Representations in the Calculation of Conformational Energies Using Small Gaussian Basis Sets, with Mezey, P. G., 134

Ratajczak, H.: Properties of Strong Hydrogen-Bonded Systems. II. *Ab initio* SCF-MO Study of the Hydrogen Bond between Nitric Acid and Ammonia, with Latajka, A., Szezesniak, M. M., and Orville-Thomas, W. J., 417

Raudino, A.: Spectroscopic CNDO/CI Study of Some Cyclic Polyenes, with Zuccarello, F., and Buemi, G., 341

Rauk, A., and Peoples, H. A.: The Electronic Structure and Optical Activity of Conjugated Dienes: 1,3-Butadiene and α- and β-Phellandrene, 240

Rothman, M. J., Bartell, L. S., Ewig, C. S., and Van Wazer, J. R.: A Pseudopotential SCF-MO Study of Te_4^{2-}, 64

Ryan, P. B.: Metal–Metal Bond Energies in Mo_2, $Mo_2Cl_8^{4-}$, and $Mo_2(O_2CH)_4$, with Norman, J. G., Jr., 59

Sannigrahi, A. B.: A Comparative Study of the Structure and Bonding of HOO, HOS, HSO, and HSS Radicals by CNDO/2 and INDO Methods, with De, B. R., 334

Scheraga, H. A.: Conformational Analysis of Proteins: Algorithms and Data Structures for Array Processing, with Pottle, C., Pottle, M. S., Tuttle, R. W., and Kinch, R. J., 46

Schweig, A., and Thiel, W.: The C_4H_4CO Potential Surface. Reactions Involving Bicyclo[2.1.0]-pentenone, 129

Seeger, R.: The Structure of Carbon Trioxide, with Pople, J. A., Seeger, U., and von Ragué Schleyer, P., 199

Seeger, U.: The Structure of Carbon Trioxide, with Pople, J. A., Seeger, R., and von Ragué Schleyer, P., 199

Shafer, S. G.: Evaluation of MINDO/3 Calculated Structures. II. Branching Errors in Alkanes and Cycloalkanes, with McManus, S. P., Smith, M. R., and Smith, M. B., 233

Smith, M. B.: Evaluation of MINDO/3 Calculated Structures. II. Branching Errors in Alkanes and Cycloalkanes, with McManus, S. P., Smith, M. R., and Shafer, S. G., 233

Smith, M. R.: Evaluation of MINDO/3 Calculated Structures. II. Branching Errors in Alkanes and Cycloalkanes, with McManus, S. P., Smith, M. B., and Shafer, S. G., 233

Sprague, J. T.: The Structures and Energies of Some Unsaturated Four-Membered Ring Carbocycles, with Allinger, N. L., and Yuh, Y., 30

—, and Allinger, N. L.: Graphite: A Molecular Mechanics Treatment, 257

Srivastava, S. K., and Mishra, P. C.: Electronic Structure of Benzaldehyde: A Comparative Study of the Lowest Excited Singlet $\pi^* \leftarrow \pi$ and $\pi^* \leftarrow n$ States, 288

Strausz, O. P.: Conformational Energy Surfaces of Triplet-State Isomeric Methyloxiranes, with DeMaré, G. R., Peterson, M. R., and Csizmadia, I. G., 141

—: A Note on Density Matrix Extrapolation and Multiple Solutions of the Unrestricted Hartree–Fock Equations, with Mezey, P. G., and Gosavi, R. K., 178

Streitwieser, A., Jr.: Integrated Spatial Electron Populations in Molecules: Application to Simple Molecules, with Collins, J. B., 81

Szezesniak, M. M.: Properties of Strong Hydrogen-Bonded Systems. II. *Ab initio* SCF-MO Study of the Hydrogen Bond between Nitric Acid and Ammonia, with Latajka, A., Ratajczak, H., and Orville-Thomas, W. J., 417

Taylor, R.: The Application of Molecular Mechanics to the Structures of Carbohydrates, with Jeffrey, G. A., 99

Tatewaki, H., and Huzinaga, S.: A Systematic Preparation of New Contracted Gaussian-Type Orbital Sets. III. Second-Row Atoms from Li through Ne, 205

Theil, W.: The C_4H_4CO Potential Surface. Reactions Involving Bicyclo[2.1.0]pentenone, with Schweig,

A., 129

Thomson, C.: Quantum Chemical Investigations of Charge Transfer Interactions in Relation to the Electronic Theory of Cancer. II, with Ball, J. R., 275

—: Quantum Chemical Investigations of Charge Transfer Interactions in Relation to the Electronic Theory of Cancer. IV. The Interaction of Formamide and the Enol Tautomers of Several Glyoxals, with Ball, J. R., 400

Trachtman, M.: An *Ab Initio* Study of the Geometry, Harmonic and Anharmonic Force Fields, and Fundamental Vibrational Frequencies of *Cis*- and *Trans*-Thiolformic Acid, with Bock, C. W., and George, P., 167

—: An *Ab Initio* Study of the Geometry and Energy of Six Planar Conformers of β-Hydroxyacrolein, with George, P., and Bock, C. W., 373

Tseng, T. J., Hong, S. H., and Whitehead, M. A.: Atomic X_α Calculations Based on $E^{\mathrm{HFS}}(\alpha) = E^{\mathrm{exp}}$, 88

Tuttle, R. W.: Conformational Analysis of Proteins: Algorithms and Data Structures for Array Processing, with Pottle, C., Pottle, M. S., Kinch, R. J., and Scheraga, H. A., 46

van Gunsteren, W. F., and Karplus, M.: A Method for Constrained Energy Minimization of Macromolecules, 266

Van Wazer, J. R.: A Pseudopotential SCF-MO Study of Te_4^{2-}, with Rothman, M. J., Bartell, L. S., and Ewig, C. S., 64

von Ragué Schleyer, P.: Isomeric Structures of Protonated Ozone: A Theoretical Study, with Kausch, M., 94

—: The Structure of Carbon Trioxide, with Pople, J. A., Seeger, U., and Seeger, R., 199

—: Small Elemental Clusters. I. The Structures of Be_2, Be_3, Be_4, and Be_5, with Whiteside, R. A., Krishnan, R., Pople, J. A., Krogh-Jespersen, M.-B., and Wenke, G., 307

Wenke, G.: Small Elemental Clusters. I. The Structures of Be_2, Be_3, Be_4, and Be_5, with Whiteside, R. A., Krishnan, R., Pople, J. A., Jespersen-Krogh, M.-B., and von Ragué Schleyer, P., 307

Whitehead, M. A.: Atomic X_α Calculations Based on $E^{\mathrm{HFS}}(\alpha) = E^{\mathrm{exp}}$, with Tseng, T. J., and Hong, S. H., 88

Whitehurst, F. W.: A Simplex Optimized INDO Calculation of ^{13}C Chemical Shifts in Hydrocarbons, with Chesnut, D. B., 36

Whiteside, R. A., Krishnan, R., Pople, J. A., Krogh-Jespersen, M.-B., von Ragué Schleyer, P., and Wenke, G.: Small Elemental Clusters. I. The Structures of Be_2, Be_3, Be_4, and Be_5, 307

Wirth, D., and Bauld, N. L.: A Theoretical Comparison of Cationic and Anionic Homoaromaticity: Reinforcement of Cationic Homoaromaticity by σ-Nonclassical Effects, 189

Wood, M. K.: Prediction of the Crystal Structure of a Cyclic Tetrapeptide, with Hall, D., 368

Yuh, Y.: The Structures and Energies of Some Unsaturated Four-Membered Ring Carbocycles, with Allinger, N. L., and Sprague, J. T., 30

Zuccarello, F., Buemi, G., and Raudino, A.: Spectroscopic CNDO/CI Study of Some Cyclic Polyenes, 341

Subject Index to Volume 1

Ab initio calculations, see also under name of compound, 59, 94, 118, 134, 141, 158, 167, 178, 181, 185, 199, 275, 281, 285, 307, 348, 358, 373, 400, 417
  charge transfer and covalency, 81
  of substituent effects, 295
Alkanes, by MINDO/3 calculations, 233
Aminoborane, 118
Aminohydroberylium, 118
Ammonia, 134
Ammonia–nitric acid, 417
Anomeric effect, 99
Array processing, 46
Atomization energies, 205

Bay regions, 149
Benzaldehyde, spectroscopic states of, 288
Benzene–chromium tricarbonyl, 407
Benzenoid hydrocarbons, 149
Beryllium, 307
Berylium, aminohydro-, 118
Berylium hydride hydroxide, 118
Bicyclo(2.1.0)pentadienone, 129
Bicyclo(2.1.0)pentenone, 129
Boron, hydroxy-, 118
Bovine pancreatic trypsin inhibitor, 46
1,3-Butadiene, 240
Butane, 181

Cancer, electronic theory of, 275
Carcinogenic hydrocarbons, 149
Carbohydrates, 192
  crystal structure–molecular mechanics comparisons, 99
  structures by molecular mechanics, 99
Carbon molecule, 205
Carbon monoxide molecule, 205
Carbon trioxide, 199
Cationic homaromaticity, 189
Charge distribution, 348
Charge transfer, 275, 400
Clusters, elemental, 307
CNDO/CI calculations, see Molecular orbital calculations
CNDO/2, see molecular orbital calculations
Computer synthesis, 323
Configuration interaction, 69, 94, 307
Conformational analysis, of proteins, 46
Conformational states, of phosphate groups, 301
Conjugated dienes, electronic structure and optical activity of, 240
Crystal structure–molecular mechanics comparisons of carbohydrates, 99
Cyclic peptide, 368
Cycloalkanes, by MINDO/3 calculations, 233
Cyclobutadiene iron–tricarbonyl complex, 407
Cyclobutene, 3, 30
1,3,5-Cycloheptatriene, 341
1,3-Cyclohexadiene, 3
1,3,5,7-Cyclononatetraene, 341
1,4,7-Cyclononatriene, 341
1,3,5,7-Cyclooctatetraene, 341
Cyclopentadienes, 21
Cyclopentadienol manganese tricarbonyl, 407
Cyclopropanone, 3

Density matrix extrapolation, 178
Dewar benzene, 3, 21, 30
Diatomic molecules, 205
Difluoroethylene, 111
Digermane, 185
Dihydroxycarbene, 158
Dihydroxymethane, 99
Dimethoxymethane, 99
Dimethylglyoxal enol, 400

Electrocyclic reaction, 3, 21
Electron correlation, 307
Electronic spectrum, of benzaldehyde, 288
Electronic transitions, 341
Electron populations, spatially integrated, 81
Electron populations, in molecules, 81
Electron projection function, 81
Energy minimization, constrained, applied to macromolecules, 266
Ethane, 81, 134
Ethylglyoxal enol, 400
Ethylmethylamine, torsional functions, 281
Ethyl methyl ether, torsional functions, 285
Extended Hückel method, see also Molecular orbital calculations, 3, 21

Fluoramine, 118
Fluorine molecule, 205
Fluoroalkenes, 111
Force field, from *ab initio* calculations, 167
Formamide, 275
Formamide-glyoxal enol, 400
Formic acid, 158
Free radicals, 334
Furan, 348, 358

Gaussian basis sets, 134
Gaussian-type orbitals, contracted, 205
Gearing, in hexamethylbenzene, 76
Germane, 185
Graph theory, 149
Graphite, molecular mechanics treatment, 257
Graph isomorphism, 386

Hartree–Fock calculations, unrestricted, 178
Heterocycles, five-membered, 348, 358
Hexamethylbenzene, 76
Homoaromaticity, 189
Hydrazine, 118
Hydrogen bonding, 417
Hydrogen cyanide, 69
Hydrogen molecule, 205
β-Hydroxyacrolein, 373
Hydroxyborane, 118
Hydroxylamine, 118
Hypofluorous acid, 118

INDO calculations, see Molecular orbital calculations
Isospectral graph, 386

Lithium amide, 118
Lithium hydroxide, 118
Lithium molecule, 205
Localized molecular orbitals, 358

Macromolecules, method for constrained energy minimization, 266
Maleic hydrazide, molecular packing of, 261
4-Membered ring, carbocycles, 30
Methanol, 81
Methoxymethanol, 99
2-Methoxytetrahydropyran, 99
Methylamine, 81
Methylberyllium hydride, 81
Methylboron hydride, 81
Methylenecyclobutane, 30
Methyl fluoride, 81
Methylglyoxal, 275
Methylglyoxal enol, 400
Methyl groups, gearing of, 76
Methyllithium, 81
Methyloxirane, 141
Methyl pyranoside, 99
Microwave plus molecular mechanics combined method, 30
MINDO/3, see also Molecular orbital calculations, 189, 233
Molybdenum–molybdenum bond energies, 59
Molecular mechanics, 30, 76, 111, 181, 192
  applications to carbohydrates, 99
  crystal structure comparisons of carbohydrates, 99
  graphite, 257
  plus microwave combined method, 30
Molecular orbital calculations, semiempirical, 3, 21, 36, 59, 88, 129, 189, 233, 334
  (X^{α}), 59, 88
Molecular orbitals, localized, 358
Moller–Plesset calculations, 307

Nitric acid–ammonia, 417
Nitrogen molecule, 205
NMR–^{13}C chemical shifts, 36

Olefins, fluorinated, 111
Optical activity, of conjugated dienes, 240
Orbital topology, 3, 21
Organic synthesis, via computer, 323
Ozone, protonated, 94

Phellandrene, 240
Phosphate groups, conformational states of, 301
Polyenes, cyclic, 341
Projection function, 81
Propanol, torsional functions, 285
Propenylglyoxal enol, 400
Propylamine, torsional functions, 281
Proteins, conformational analysis of, 46
Proteins, folding of, 46
Protonated ozone, 94
Pseudopotential SCF method, 59
Pyranose rings, 99
Pyrrole, 348, 358

Random walks, 386
*t*RNA, crystal structure of, 301

Semiempirical calculations, see Molecular orbital calculations
Sigma-nonclassical effects, 189
Substituent effects, 118, 295
Synthesis, via computer, 323

Tetraoxabicyclo(4.4.0)decane, 192
Tetraoxabicyclo(5.3.0)decane, 192
Tetratellurium (II), *ab initio* calculations, 59
Thiolformic acid, 167
Thiophene, 348, 358
Topology, orbital, 3, 21
Torsional potential functions, 181, 185, 281, 285
Transition metal tricarbonyls, 407
Transition state calculations, 158
Trimethylenemethane iron–tricarbonyl complex, 407
Trioxirane, 94
Triplet states, 141
Trypsin inhibitor, 46

Valence and core representations, in *ab initio* calculations, 134

Woodward–Hoffmann rules, 3, 21, 129, 158